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# **Improving Water Quality Index Prediction in Perak River Basin Malaysia through the Combination of Multiple Neural Networks**

Ahmad, Z<sup>a,\*</sup>, N A Rahim<sup>a</sup>, Alireza Bahadori<sup>b</sup>, Jie Zhang<sup>c</sup>

<sup>a</sup>School of Chemical Engineering, University Sains Malaysia, Engineering Campus, Seri Ampangan, 14300, Nibong Tebal, Penang, Malaysia

E-mail: chzahmad@usm.my

<sup>b</sup>School of Environment, Science and Engineering, Southern Cross University, Lismore NSW Australia.

Email: Alireza.Bahadori@scu.edu.au

<sup>c</sup>School of Chemical Engineering and Advanced Materials, Newcastle University, Newcastle upon Tyne NE1 7RU, UK

E-mail: jie.zhang@newcastle.ac.uk

## **Abstract**

This paper proposes a method for the real-time prediction of water quality index by excluding the biological oxygen demand and chemical oxygen demand, which are not measured in real-time, from the model inputs. In this study, feedforward artificial neural networks are used to model the water quality index in Perak River Basin Malaysia due to its capability in modelling nonlinear systems. The results show that the developed single feed forward neural network model can predict water quality index very well with the coefficient of determination  $R^2$  and mean squared error (MSE) of 0.9090 and 0.1740 on the unseen validation data respectively. In addition to that, the aggregation of multiple neural networks in predicting the water quality index further improves the prediction performance on the unseen validation data. Forward selection and backward elimination selective combination methods are used to

combine multiple neural networks and both methods leads to 6 and 5 networks being combined with  $R^2$  and MSE of 0.9340, 0.9270 and 0.1156, 0.1256 respectively. It is clearly shown that combining multiple neural networks does improve the performance for water quality index prediction.

Keywords: Water Quality Index, Feedforward Artificial Neural Network, Forward Selection, Backward Elimination, Artificial Neural Network, Multiple Neural Networks

## **1. Introduction**

The environmental preservation efforts, especially on water quality and air quality, have attracted more and more attention. In the last decades, many researchers have monitored the gradual accumulation of long-term environmental quality data (Antonopoulos et al. 2001). Environmental quality prediction has received more attention as it plays an important role in the control, management and planning of agriculture and aquaculture activities (Dhalla et al.,2008). Water quality is one of the main aspects in the environmental management and water is becoming the major constraining resource for sustainable development of large areas in the world.

Different regions have different specifications for water quality index (WQI). The WQI for individual regions or countries is recommended by their own authorities, such as Interim National Water Quality Standard for Malaysia, British Columbia WQI, Canadian Water Quality Index (CWQI), and National Sanitation Foundation WQI (NSF WQI). Each of these WQI differs from others in terms of variables and parameters involved in its calculation. To the best of our knowledge, a unified environmental quality index like WQI has not been reported or developed yet. The complexity of models has to be compatible with the quantity and quality of available environmental data (Loucks and Beek,2005). The developed environmental quality model should also have been opted to have the most meaningful and

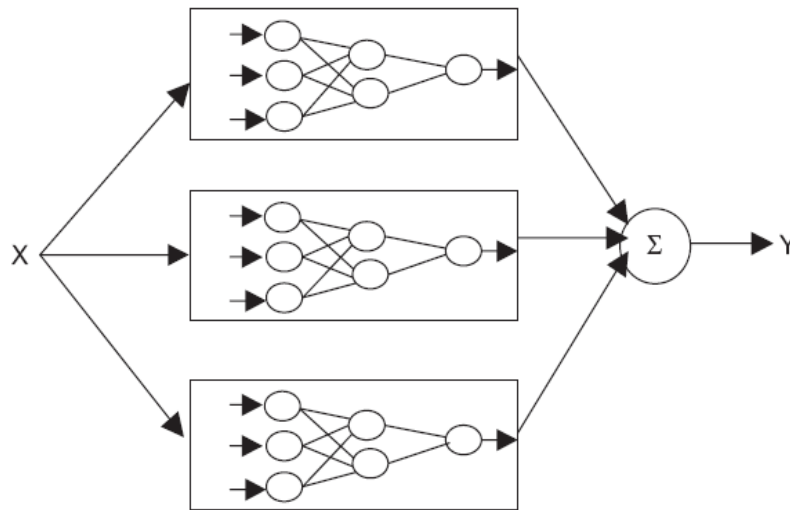
understandable response to the communities; either to inform about the pollutant sources or water quality conditions (Thoe et al., 2014).

According to Boyacioglu (2006), a basic problem in the case of water quality monitoring is the complexity associated with analyzing the large number of variables. Artificial Intelligence (AI) approaches as predicting tools have also been applied for water and environmental quality studies (Li and Hassan, 2006). One of the most popular AI methods is artificial neural networks (ANN) or feedforward neural networks (FANN) which are inspired from the neurological system of humans and intended to mimic the human neurological system. ANN has shown remarkable successes in the modelling and prediction of highly nonlinear systems including water quality prediction cases (Khuan et al., 2002). In some cases, the modelling using ANN is combined with other statistical analysis tools to improve the model performance like what has been done by Cho et al. (2011) where ANN is combined with principal component regression (PCR) to predict the ground water arsenic content and the result shows that PCR-ANN did improve the prediction. This combination of tools for ANN model prediction has also been applied by other researchers to enhance the ANN model performance (Han et al., 2011; Faruk, 2010; Khan et al., 2001; Xu and Liu, 2013). This clearly shows that in some situations, ANN needs additional tools to improve the model robustness especially when dealing with real world data like water quality prediction which typically contain a lot of noise in data sampling.

The greatest strength of neural network is that it has the ability to learn the system from its historical data. It has emerged out to be a more flexible, less assumption dependent and adaptive methodology in environmental related areas such as water quality and air quality management, lake and reservoir modelling, hydrologic forecasting and others. Rabiatal and Zainal (2012) demonstrate that the main advantage of neural network based

process models is that they are easy to build. This feature is particularly useful when modelling complicated processes where detailed mechanistic models are difficult to develop.

However, single neural networks sometimes lack robustness when the data is insufficient especially when dealing with real world data due to the fact that the robustness of the network is related to the representativeness of the training data (Bishop, 1995). Single neural networks sometimes suffer badly when applied to unseen data where some neural networks might fail to deliver the correct result due to the network training converged to undesired local minima or overfitting of noise in the data (McLoone and Irwin, 2001). Therefore the combination of multiple neural networks is proposed in this paper with the aim of enhancing the neural network robustness for environmental quality prediction. There are several types of multiple neural networks but their underlying ideas are basically similar and the main difference is on how to create the sub-models. Figure 1 shows the combination of multiple neural networks.



**Fig. 1** Combining multiple neural networks

In this study, the multiple neural network models are created using the same training data but re-sampled using bootstrap re-sampling approach (Zhang et al., 1998; Zhang, 1999).

The motivation of creating those different training data sets is to create the effective network ensembles where the individual networks differ. In a bootstrap replication of the training data, some of the original data samples may occur several times, and other may not occur in the replication at all. In this paper, selective combination of neural networks is carried out using forward selection (FS) and backward elimination (BE) approaches (Ahmad and Zhang, 2009). The outputs from the selected multiple models are linearly combined to produce the final prediction.

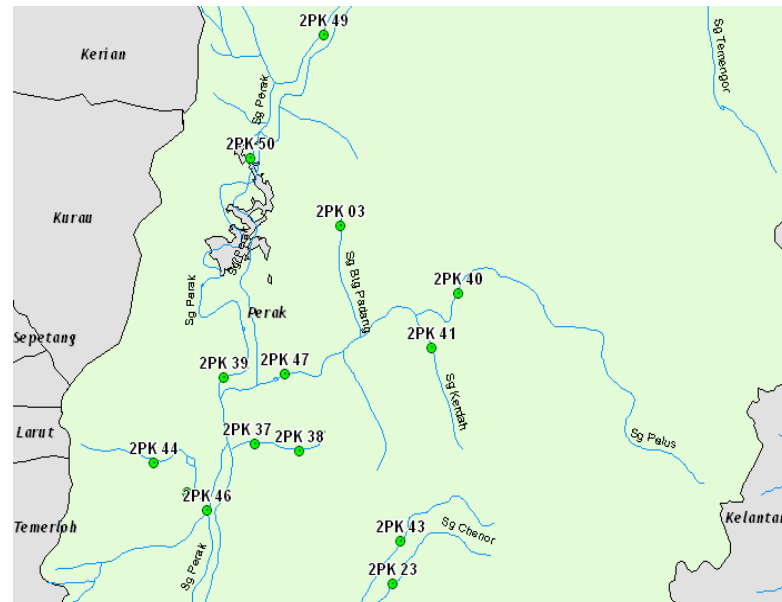
This paper is organized as follows. Section 2 presents the case study. The concept of feedforward neural network and multiple neural network modelling is presented in Section 3. The results and discussions of the proposed WQI modelling method are presented in Section 4. Finally, the last section concludes this paper.

## **2. Materials and methods**

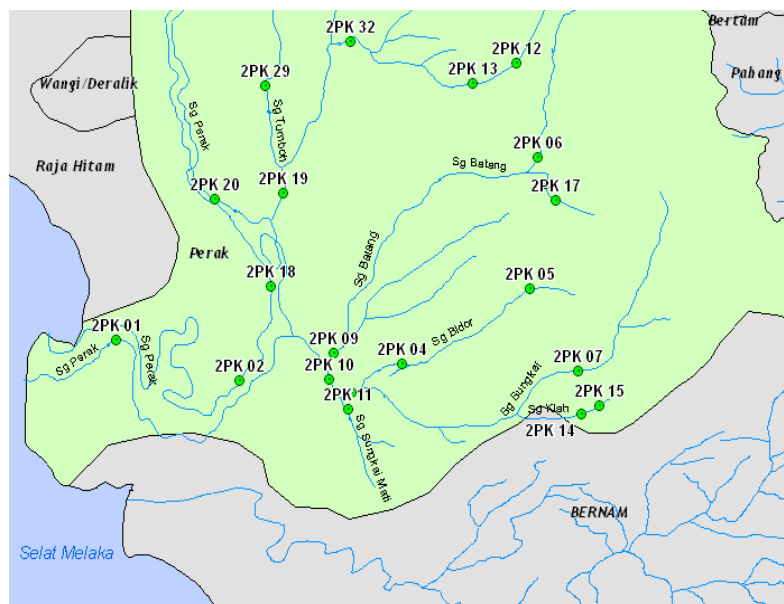
### **2.1 Perak River Basin: Water Quality Monitoring Station**

The case study is situated in the state of Perak, Malaysia, where there are 11 major river basins that cover over 80 square kilometres. The Perak River basin is about 760 km long with an area of 14,908 km<sup>2</sup>. Perak River basin, shown in Figures 2, 3 and 4, is the biggest river basin in this area, which covers about 70% of state area. If water in the Perak River basin is contaminated it will affect most of the river basin in Perak State and affect the human population as well as the financial income of the local population where most of the activity in this area is fishing and agricultural activities. The purpose of the case study is to predict the water quality of the Perak River basin in real time. If poor river water quality is predicted, some preventive measures can be taken immediately. The sample and data collection was duly carried out by the Department of Environment (DOE) of Malaysia through Alam Sekitar Malaysia Sdn. Bhd (ASMA, 2012). The concerned area in the Perak river basin is divided

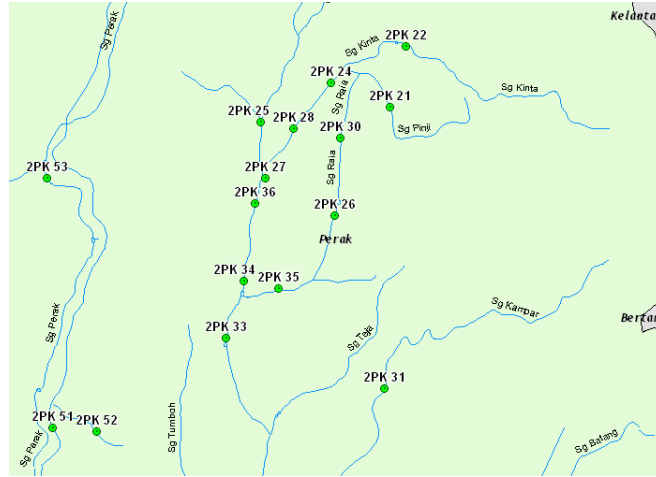
into 3 sections which are north, south and central areas as shown respectively in Figures 2, 3, and 4 and it covers 21 rivers along the Perak river basin. The samples are taken daily in some points using automatic sampling approach and at some points they are manually taken once a week or twice a month.



**Fig. 2** Perak (North) river basin monitoring stations (ASMA, 2012)



**Fig. 3** Perak (South) river basin monitoring stations (ASMA, 2012)



**Fig. 4** Perak (Central) river basin monitoring stations (ASMA, 2012)

The DOE of Malaysia introduced the WQI monitoring approach in 1978. The approach considers six variables, which are dissolved oxygen (DO), biological oxygen demand (BOD), chemical oxygen demand (COD), suspended solid (SS), the pH value (pH), and ammonical nitrogen ( $\text{NH}_3\text{-NL}$ ) (Khuan et al., 2002). DOE applies the following formula for the calculation of WQI (Mamun et al., 2009):

$$\text{WQI} = 0.22\text{SI}_{\text{DO}} + 0.19\text{SI}_{\text{BOD}} + 0.0.16\text{SI}_{\text{COD}} + 0.16\text{SI}_{\text{SS}} + 0.15\text{SI}_{\text{AN}} + 0.22\text{SI}_{\text{pH}} \quad (1)$$

Where,

WQI = Water quality index;  $\text{SI}_{\text{DO}}$  = Sub-index of DO;  $\text{SI}_{\text{BOD}}$  = Sub-index of BOD;  $\text{SI}_{\text{COD}}$  = Sub-index of COD;  $\text{SI}_{\text{AN}}$  = Sub-index AN;  $\text{SI}_{\text{SS}}$  = Sub-index of TSS;  $\text{SI}_{\text{pH}}$  = Sub-index of pH.

The in-situ measurements by DOE are DO (mg/l), turbidity (NTU), conductivity (uS/cm), salinity (ppt), pH and temperature. The remaining chemical and biological parameter analysis are carry out in the laboratory. Therefore, in this study, BOD and COD variables are not used for the real time prediction of WQI due to the reason that BOD takes at least 5 to 7 days ( $\text{BOD}_5$  or  $\text{BOD}_7$ ) to get the result and COD takes several hours to get the result from the



analysis. An FANN model will be developed to get more accurate and faster WQI predictions variables shown in Table 1.

**Table 1.** Summary of the input and output variables for WQI Prediction

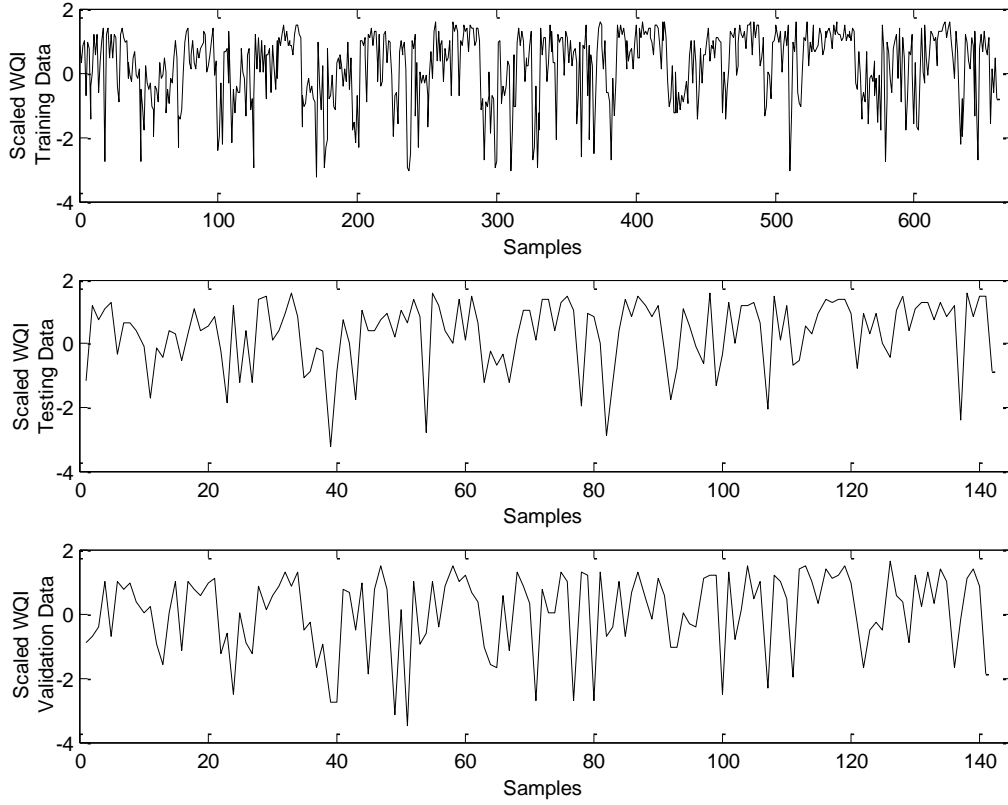
Inputs	DO, SS, pH, NH <sub>3</sub> -NL, TEMP, COND, TUR, DS, TS, NO <sub>3</sub> , Cl, PO <sub>4</sub> , As, Zn, Ca, Fe, K, Mg, Na, OG, E-Coli, Coliform, Cd, Cr, Pb
Output	WQI

## 2.2 Feedforward Artificial Neural Network Model Development

In this case study, 942 samples are taken from the DOE of Malaysia database from year 2000 to year 2004. All the data are normalized to zero mean and unit standard deviation to cope with the different magnitudes in the input and output data. Then, the input data are divided randomly using Matlab<sup>TM</sup> command *divideint* into three sets of data which are 70% (659 samples) for training, 15% (142 sample) for testing, and 15% (141 samples) for unseen validation as shown in Figure 5. Then the individual networks are trained by the Levenberg-Marquardt optimization algorithm with regularization and “early stopping”. All network weights and biases are randomly initialized in the range from  $-0.1$  to  $0.1$ . The networks are single hidden layer FANN. The hidden layer neurons use the logarithmic sigmoid activation function whereas the output layer neurons use the linear activation function.

The number of hidden neurons is determined using cross validation. The number of hidden nodes is increased from 1 to 15 and the corresponding mean squared errors (MSE) and  $R^2$  values for the training and testing data are calculated. Then, the MSE and  $R^2$  values are plotted against the number of hidden nodes. The network with the lowest MSE value on

the training and testing data is considered as having the best network topology. In addition, in assessing the developed models, MSE on the unseen validation data is used as the performance criterion.



**Fig. 5** Training, testing and validation data for WQI FANN model development

For this case study, the FANN is developed based on the discrete time of the process as the prediction output at time  $t$ ,  $y(t)$ , is predicted based on the process input at time  $t$ ,  $u(t)$ , as follows:

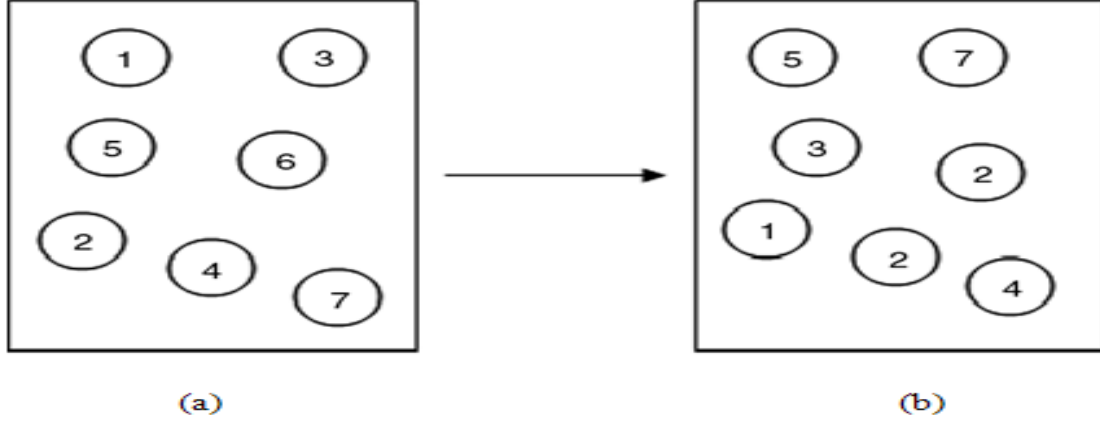
$$\hat{y}(t) = f[u_1(t), u_2(t), \dots, u_m(t)] \quad (2)$$

where  $u_i(t)$  is the  $i$ th process input at time  $t$ ,  $\hat{y}(t)$  is the predicted process output (WQI) at time  $t$ , and  $m$  is the number of neural network model inputs which for this case study is 25 as shown in Table 1.

### 2.3 Bootstrap Re-sampling Approach

In this study, bootstrap re-sampling basically refers to replication of a training data set through random re-sampling the original training data set. Some of the data samples in the original data set may occur several times and some other samples may not occur in the replication at all. The individual training sets are independent and the neural networks can be trained in parallel. Combining multiple neural networks trained on bootstrap re-sampled data does actually increase the robustness of the model. Bootstrap technique also can generate diverse networks when the base learning algorithm is unstable in that small changes in the training data set will cause large changes in the learned model while boosting can result in less instability. Figure 6 illustrates the analogy of bootstrap re-sampling technique. The numbers in the box represent the sample number (Zhang, 1999).

Here, 20 networks with fixed identical structure are developed from bootstrap re-sampling replications of the original training and testing data. The rationale to choose 20 networks for all combination is based on the work of Zhang (1999) which shows that constant MSE is generally observed after combining about 15 networks. Therefore combining 20 neural networks would be reasonable. If the number of networks is too small we might not get the optimum reduction of the SSE in the combination. In re-sampling the training and testing data using bootstrap re-sampling technique, the training and testing data are first transformed in the form corresponding to the discrete time functions as shown in Eq.(2) in model inputs and outputs, therefore re-sampling the transformed data does not affect the input-output mapping of the models.



**Fig. 6** Bootstrap re-sampling: (a) Data samples in the original data set; (b) Data samples in the re-sampled data set.

#### 2.4 Forward Selection and Backward Elimination with Simple Averaging

In order to develop an aggregated neural network model containing  $n$  individual networks, the original data set can be re-sampled using bootstrap re-sampling with replacement to form  $n$  replications of the original data set (Zhang, 1999; Ahmad and Zhang, 2009). The  $n$  replications can be denoted as  $\{X_{(1)}, Y_{(1)}\}, \{X_{(2)}, Y_{(2)}\}, \dots, \{X_{(n)}, Y_{(n)}\}$ , where  $X_{(i)} \in R^{N \times p}$ ,  $Y_{(i)} \in R^{N \times q}$ ,  $i=1, 2, \dots, n$ . A neural network model can be developed on each of these replications, which can be partitioned into a training data set and a testing data set if cross-validation is used in network training and network structure selection. If the predictions of these  $n$  networks on the original data set are denoted as  $\hat{Y}_1, \hat{Y}_2, \dots, \hat{Y}_n$ , then the mean sum of squared errors (MSE) of the  $i$ th network can be calculated as

$$SSE_i = \text{trace}[(Y - \hat{Y}_i)^T (Y - \hat{Y}_i)] \quad (3)$$

$$MSE_i = SSE_i / m$$

Where  $m$  is number of samples

The simple average method is used in combining the selected networks as shown in Eq (4) where if all  $n$  networks are combined, then the aggregated network output is:

$$\hat{Y} = \frac{1}{n} \sum_{i=1}^n \hat{Y}_i \quad (4)$$

The FS and BE methods were developed in our previous paper (Ahmad and Zhang, 2009) and are briefly introduced here. Generally, in FS, individual networks are added one at a time to the aggregated network. This process starts with an empty aggregated model and the first network to be added to the aggregated network is the single network that has the least MSE in training and testing data or what can be called the best individual network. The second network to be added is the one, when combined with the first added network, produces the largest reduction in MSE on the original training and testing data. This procedure is repeated until the MSE on the training and testing data cannot be further reduced by adding more networks. On the other hand, in the BE method, the aggregated network begin with combining all the individual networks and removes one network at a time until the MSE on the training and testing data cannot be further reduced. The network deleted at each step is such selected that its deletion results in the largest reduction in the aggregated network MSE on the training and testing data. The detailed procedures for FS and BE methods can be found in Ahmad and Zhang (2009).

### **3. Results and Discussions**

#### **3.1 Single FANN Model Prediction**

In Table 2, the performances of FANN WQI prediction in terms of MSE are tabulated with different numbers of hidden neurons. Selection of an appropriate number of nodes in the hidden layer is important as a larger number of hidden nodes may result in over-fitting, while

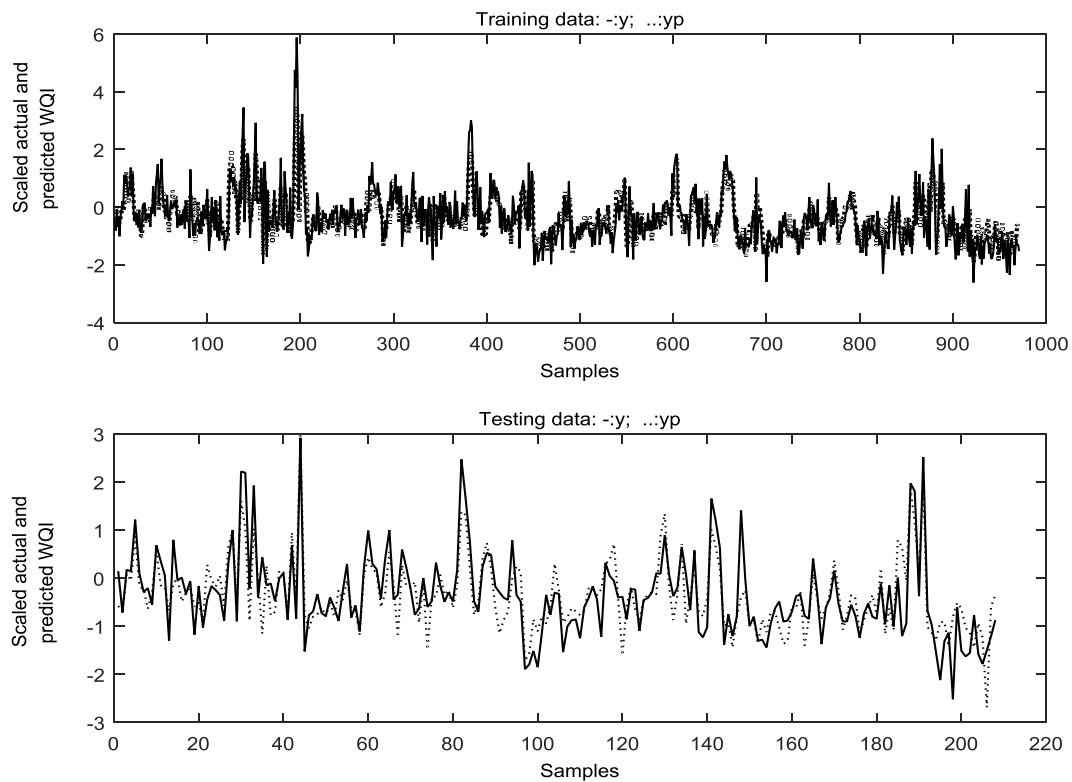
a smaller number of hidden nodes may not capture the information adequately. The lowest value of the combined MSE on training and testing data is the criteria to choose for the final number of hidden neurons. As shown in Table 2, network with 12 hidden neurons has the best performance in WQI prediction. The combined MSE value of 0.0575 on both training and testing data sets is the lowest among all the considered networks. Therefore each network is assigned with 12 neurons in the hidden layer for good model generalization capability.

Figures 7 and 8 shows the performance of the FANN with 12 hidden neurons. Figure 7 shows the actual (solid line) and predictions (dashed line) on the training and testing data. Figure 8 shows the actual (solid line) and predictions (dashed line), as well as model residues, on the unseen validation data. Figures 7 and 8 clearly show that the performance of the FANN model is good as the model predictions are close to the actual values of WQI. As shown in these figures, the network possesses the ability to generalize and adapt to the new input data. As shown in Figure 8, the FANN model performance for predicting WQI on the unseen validation data is good, which is also supported by the statistical analysis result shown in Table 3. The  $R^2$  values is more than 0.9 and the p-values is so significant which is lower than 0.05 and the MSE value of 0.1740 is relatively small.

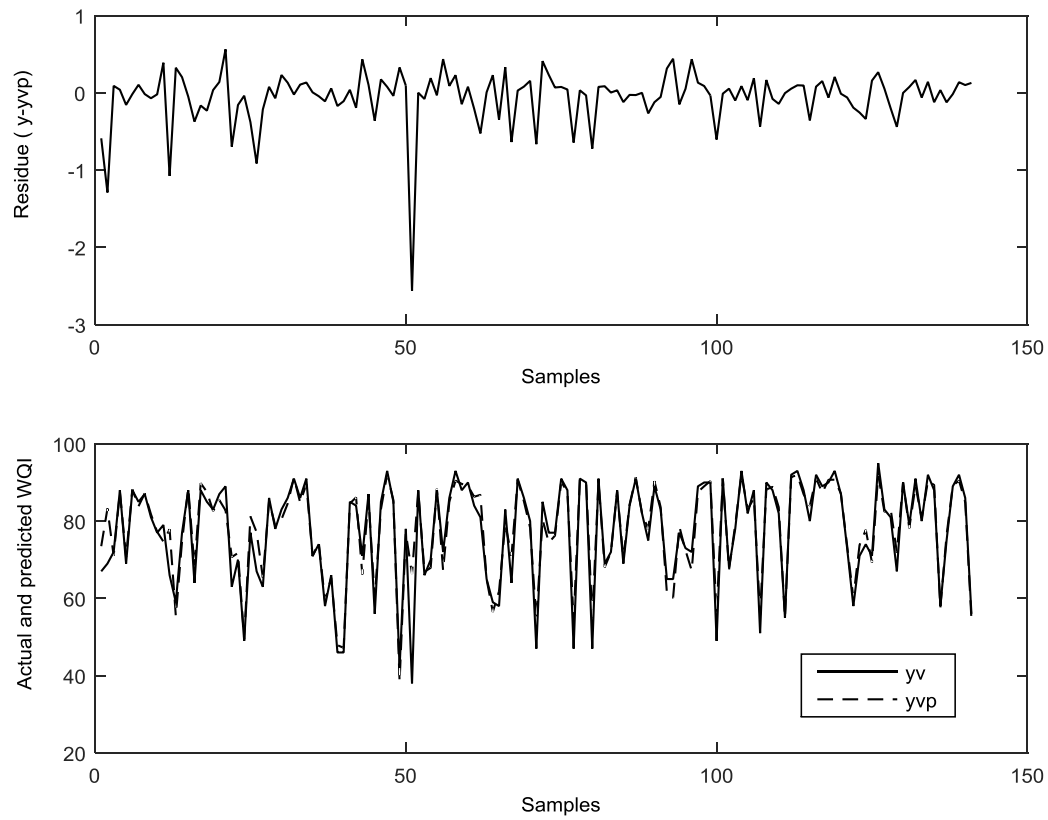
**Table 2.** MSE for different numbers of hidden neurons in WQI prediction

No of nodes	MSE (Train)	MSE (Test)	MSE (Train + Test)
1	0.0474	0.1392	0.0637
2	0.1029	0.1136	0.1048
3	0.0941	0.0997	0.0951
4	0.0974	0.1060	0.0989
5	0.0639	0.1098	0.0720

6	0.0588	0.0843	0.0633
7	0.0986	0.0907	0.0972
8	0.0626	0.1347	0.0754
9	0.1088	0.1218	0.1111
10	0.1058	0.1415	0.1121
11	0.0787	0.0993	0.0824
<b><u>12</u></b>	<b><u>0.0461</u></b>	<b><u>0.1103</u></b>	<b><u>0.0575</u></b>
13	0.0709	0.0822	0.0729
14	0.0906	0.1015	0.0925
15	0.1012	0.1149	0.1036



**Fig. 7** Actual and predicted values on the training and testing data



**Fig. 8** Actual and predicted values on the unseen validation data for single FANN

Table 3-Statistical analysis for model performance on the unseen validation data

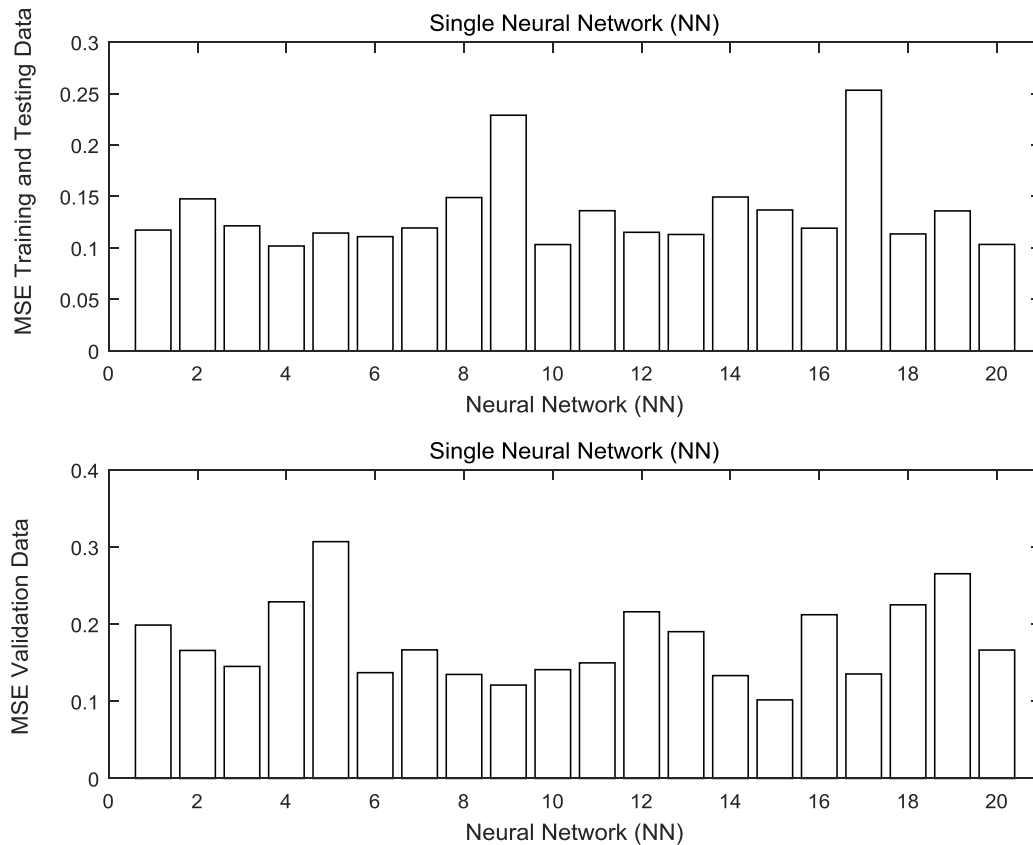
Details	Values
$R^2$	0.9090
MSE	0.1740
$p$ -value	$3.148 \times 10^{-74}$

### 3.2 Multiple Neural Network Model

To further enhance model performance, bootstrap aggregated neural networks are developed. In this case study, 20 networks are developed using bootstrap re-sampling replications of the original training and testing data. Figure 9 shows the performance of individual networks on

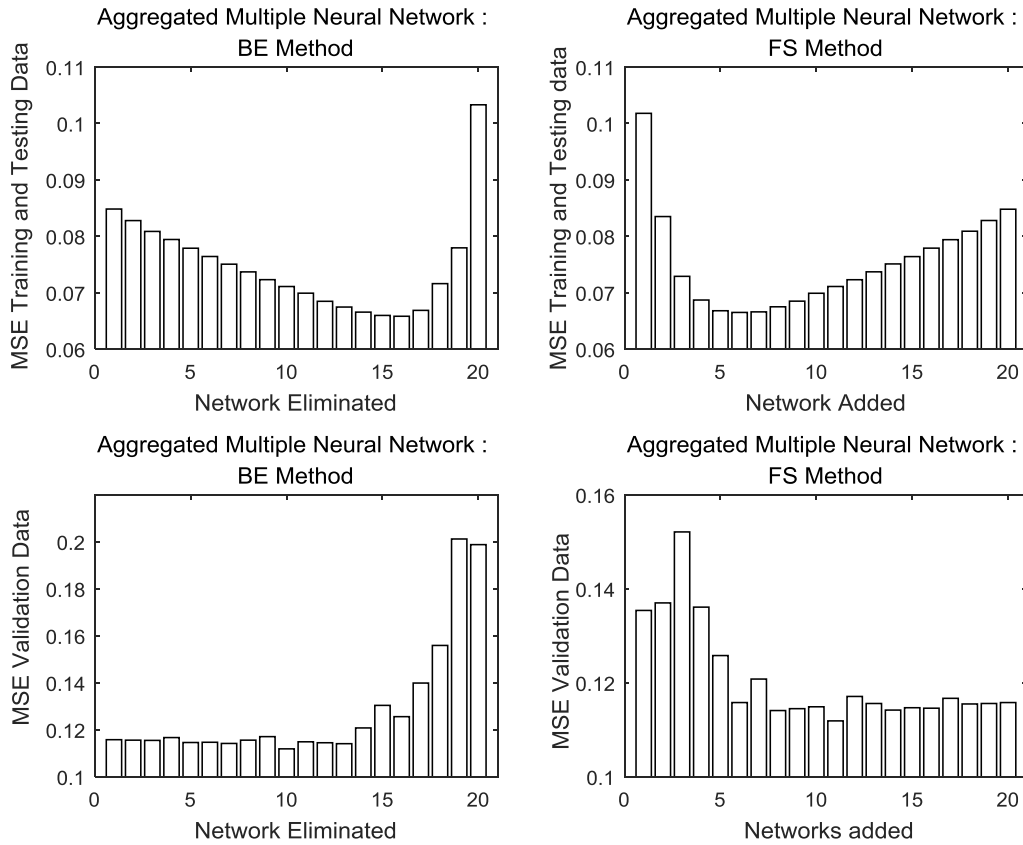


the training, testing, and unseen validation data. It can be seen that the performance of individual neural networks varies quite significantly. The performance on training and testing data sometimes does not reflect the performance on the unseen validation data. The best performance on training and testing data for this case is from network no. 10, however it does not give the best performance on the unseen data, where network no. 9 is the best on the unseen data. This demonstrates the different, and sometimes quite poor, generalisation capabilities of individual networks and also the non-robust nature of individual neural networks. Once these individual networks are developed, they are combined using BE and FS combination schemes through simple averaging.



**Fig. 9** Performance of individual neural networks on training, testing and validation data

Figure 10 shows the FANN model prediction performance of the aggregated neural networks with selective combination using BE and FS methods. It is clearly shown that under both the FS and BE approaches, the reduction of MSE on the training and testing data is quite consistent with the reduction of MSE on the unseen validation data. As shown in Table 4, only 5 and 6 networks are combined for BE and FS methods respectively. The  $R^2$  and MSE values for BE and FS are 0.9270, 0.9390 and 0.1200, 0.1158 respectively. The performance is slightly better than the best individual network and combining all networks which have  $R^2$  and MSE values of 0.9090, 0.9310 and 0.1740, 0.1159 respectively.



**Fig. 10** MSE of aggregated multiple neural networks using BE and FS approaches

It should be noticed that, although the selective combination methods combined only 5 and 6 networks, their performance is still better than a single and combining all the

networks. This clearly demonstrates that the aggregated neural network models are more robust compared to single a neural networks, furthermore, the selective combination gives better performance than combining all the networks.

The most significant finding from this study is by the exclusion of COD and BOD from the input of the model prediction for single FANN and MNN, it does not have much effect to the WQI final performance prediction. This finding was supported by the performance of the new model shows in Figure 8, Figure 10 and Table 4.

Table 4-Statistical analysis for unseen validation data for multiple neural networks

	No of network combined	MSE	$R^2$
Single FANN	1	0.1740	0.9090
Combined all MNN	20	0.1159	0.9310
FS Aggregated MNN	6 (2,4,10,13,16,20)	0.1156	0.9340
BE Aggregated MNN	5 (2,10,13,16,20)	0.1256	0.9270

#### 4. Conclusions

A reliable real-time prediction model for water quality index is developed through selective combination of multiple neural networks by excluding COD and BOD from model inputs as they cannot be measured in real-time. Single and multiple feedforward artificial neural networks are used in this paper to model the water quality index in Perak River basin. The conclusions of this study are listed as below:

1. The results show that the developed FANN model is able to give good real-time prediction performance for WQI with the exclusion of BOD and COD from the model input variables.
2. In order to overcome the non-robust nature of single FANN in the prediction, multiple neural networks are used and they give better prediction performance as compared to single FANN models.
3. The selective combination schemes provide models with better generalization capability compared to combining all neural networks.

The bootstrap aggregated models with selective combination provide a real-time WQI prediction tool without delay as only real-time measurements are used as model inputs. This tool will greatly improve the mitigation activity in the river and speed up the action taken by the local authority or DOE Malaysia. This is very important due to the fact that the main activities in this area are fisheries and agricultural activity that solely depends on the river water quality.

### **Acknowledgement**

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## **Nomenclature**

AI	Artificial Intelligence
ANN	Artificial Neural Network
As	Arsenic, mg/l
ASMA	Alam Sekitar Malaysia Sdn. Bhd.
BE	Backward Elimination
BOD	Biological Oxygen Demand, mg/l
BP	Back Propagation
Ca	Calcium, mg/l
Cd	Cadmium, mg/l
COD	Chemical Oxygen Demand, mg/l
Coliform	Total coliform, MMPN
Cond	Conductivity, uS/cm
Cl	Chlorine, mg/l
Cr	Chromium, mg/l
DO	Dissolved Oxygen, mg/;
DOE	Department of Environment

DS	Dissolved solid, mg/l
E-coli	Faecal coliform, MPN
FANN	Feedforward Artificial Neural Networks
Fe	Iron, mg/l
INWQS	Interim National Water Quality Standards
K	Potassium, mg/l
MISO	Multi Input Single Output
Mg	Magnesium, mg/l
MLP	Multiple Layer Perceptron
MNN	Multiple Neural Network
MSE	Mean Square Error
Na	Natrium, mg/l
NH <sub>3</sub> -NL	Ammoniacal nitrogen, mg/l
NO <sub>3</sub>	Nitrate, mg/l
OG	Oil and Grease, mg/l
Pb	Plumbum, mg/l
PCR	Principal Component Regression
pH	pH



PO <sub>4</sub>	Phosphate, mg/l
R <sup>2</sup>	Coefficient determination
Sal	Salinity, ppt
SI <sub>DO</sub>	Sub-index of DO
SI <sub>BOD</sub>	Sub-index of BOD
SI <sub>COD</sub>	Sub-index of COD
SI <sub>AN</sub>	Sub-index AN
SI <sub>SS</sub>	Sub-index of TSS
SI <sub>pH</sub>	Sub-index of pH
SS	Suspended Solid, mg/l
SSE	Sum Square Error
TEMP	Temperature , C
Tur	Turbidity, NTU
WQI	Water Quality Index
Zn	Zink, mg/l